Diethyl sulfate

64-67-5 | DTXSID1024045

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 208 °C

Global applicability domain: Inside

Local applicability domain index: 5.20e-01

Confidence level: 6.07e-01

Nearest Neighbors from the Training Set

Image not found
Diethyl sulfate
Measured: 208
Predicted: 208

Image not found
2-Chloro-ethanesulfonyl chloride
Measured: 202
Predicted: 203

Image not found
Sulfolane
Measured: 285
Predicted: 263

Image not found
Sulfurous acid, diethyl ester
Measured: 158
Predicted: 170